I'm trying to calculate the diffusion coefficient of lipids in a bilayer using:

gmx msd -lateral z -f test.xtc -n index.ndx -s topol.tpr -o msd.xvg -rmcomm -mol diff.xvg

I select group "POPC" to calculate mean squared displacement and group "Membrane" for center of mass removal. The program stalls or segfaults while reading the first frame. To me it looks like the code is trying to calculate the COM of "Membrane" using the COM coordinates of POPC molecules (xa[prev] instead of x[prev]).

I tried to fix the problem using small modifications shown below, but I'm not sure if the center of mass is calculated correctly. The results seem to be OK though.

```bash
$ diff gmx_msd.cpp_fixed gmx_msd.cpp_original
802,803c802,803
<       prep_data(false, gnx_com[0], index_com[0], x[cur], x[prev], box);
<       calc_com(false, gnx_com[0], index_com[0], x[cur], x[prev], box,
---
>       prep_data(bMol, gnx_com[0], index_com[0], xa[cur], xa[prev], box);
>       calc_com(bMol, gnx_com[0], index_com[0], xa[cur], xa[prev], box,
```

Associated revisions

Revision 0a5e6f65 - 01/04/2018 11:13 AM - Paul Bauer
Fix gmx msd when using COM removal and molecules

Changed order of code to actually assign correct coordinates before copying the data, and modified data structure size when using COM removal and individual molecules.

Fixes #2043

Change-Id: lc16f05a589609a43f14fd75753ca8589cf3d8c42

History

#1 - 12/20/2016 09:24 PM - Chris Neale
I can confirm that I see this with gromacs 5.1.2 for two different test systems. More details are below, but basically as originally reported there is an infinite hang at the start when -mol is combined with -rmcomm.

I find that gmx msd (version 5.1.2) hangs when I use the -rmcomm option. If I run a test like this:

```bash
#!/bin/bash
gro=EQUIL.gro
xtc=MD.xtc
tpr=MD.tpr
rm -f tmp.ndx
gmx make_ndx -f $gro -o tmp.ndx << EOF
r1
r1-60
q
```
rm -f msd.xvg diff_mol.xvg
echo -e "r1\nr_1-60\n" | gmx msd -s $tpr -f $xtc -n tmp.ndx -o msd.xvg -mol diff_mol.xvg -lateral z -rmcomm -e 100

Then it hangs forever after outputting:

<<... snip ...>>
Command line:
  gmx msd -s MD.tpr -f MD.xtc -n tmp.ndx -o msd.xvg -mol diff_mol.xvg -lateral z -rmcomm -e 100

Calculating diffusion coefficients for molecules.
Reading file MD.tpr, VERSION 5.1.2 (single precision)
Reading file MD.tpr, VERSION 5.1.2 (single precision)

Select a group to calculate mean squared displacement for:
Group 0 (System) has 17248 elements
Group 1 (Other) has 8280 elements
Group 2 (DOPC) has 8280 elements
Group 3 (K) has 8 elements
Group 4 (CL) has 8 elements
Group 5 (Water) has 8952 elements
Group 6 (SOL) has 8952 elements
Group 7 (non-Water) has 8296 elements
Group 8 (Ion) has 16 elements
Group 9 (DOPC) has 8280 elements
Group 10 (K) has 8 elements
Group 11 (CL) has 8 elements
Group 12 (Water_and_Ions) has 8968 elements
Group 13 (r_1) has 138 elements
Group 14 (r_1-60) has 8280 elements
Select a group: Selected 13: ’r_1’

Now select a group for center of mass removal:
Group 0 (System) has 17248 elements
Group 1 (Other) has 8280 elements
Group 2 (DOPC) has 8280 elements
Group 3 (K) has 8 elements
Group 4 (CL) has 8 elements
Group 5 (Water) has 8952 elements
Group 6 (SOL) has 8952 elements
Group 7 (non-Water) has 8296 elements
Group 8 (Ion) has 16 elements
Group 9 (DOPC) has 8280 elements
Group 10 (K) has 8 elements
Group 11 (CL) has 8 elements
Group 12 (Water_and_Ions) has 8968 elements
Group 13 (r_1) has 138 elements
Group 14 (r_1-60) has 8280 elements
Select a group: Selected 14: ’r_1-60’
Split group of 138 atoms into 1 molecules
Reading frame 0 time 0.000
However, if I remove the -rmcomm option and run like this:
echo -e "r1\n" | gmx msd -s $tpr -f $xtc -n tmp.ndx -o msd.xvg -mol diff_mol.xvg -lateral z -e 100

there it is fine:

<<... snip ...>>
Select a group: Selected 13: ’r_1’
Split group of 138 atoms into 1 molecules
Last frame 50 time 100.000

Used 11 restart points spaced 10 ps over 100 ps

<D> = 0.0329 Std. Dev. = 0.0000 Error = 0.0000
Fitting from 10 to 90 ps
D[r_1] 0.0308 (+/- 0.0149) 1e-5 cm^2/s

gcq#494: "If it's a good idea, go ahead and do it. It's much easier to apologize than it is to get permission."
(Grace Hopper, developer of COBOL)
The hang with -rmcomm still exists even if I don't use the "-lateral z" option is removed, but removing -mol fixes the problem.

#2 - 01/03/2018 01:34 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #2043.
Uploader: Paul Bauer (paul.bauer.q@gmail.com)
Change-Id: gromacs~release-2018~Ic16f05a589609a43f14fd75753ca8589cf3d8c42
Gerrit URL: https://gerrit.gromacs.org/7423

#3 - 01/03/2018 02:04 PM - Erik Lindahl
- Target version set to 2018

#4 - 01/03/2018 08:10 PM - Erik Lindahl
- Status changed from New to Fix uploaded

#5 - 01/04/2018 04:20 PM - Mark Abraham
- Status changed from Fix uploaded to Closed
- Assignee set to Paul Bauer

Files

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